Theory of the cross sections for inelastic scattering of electrons by core level excitations in solids

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Abstract

A calculation of cross sections for the inelastic scattering of electrons from core levels is carried out based on a model in which core level electrons are excited into a free-electron-like band state. A simplified model is also developed that assumes oscillator strengths appropriate to band-to-band excitations in solids. The results for Al L_{23} and Mo M_{45} cross sections are compared with a number of previous calculations. These previous calculations include: (a) the constant-oscillator-strength model, (b) the Rez model (based on excitations to atomic-like states), and (c) the semi-empirical hydrogenic model proposed by Egerton. We have incorporated optical data into all of the models considered in this paper with the exception of Egerton's. Calculations are presented for incident electron energies of 100, 200 and 500 keV, collection angles of 1–41 mrad, and energy collection windows of 20–200 eV. Comparison is also made with experiment where possible and reasonable agreement is found.

1. Introduction

A discussion of the factors affecting the accuracy of elemental analysis by electron energy-loss spectroscopy has been given by Egerton [1]. A key ingredient is knowledge of the inelastic scattering cross sections for excitations from the core levels in solids. Previous theoretical calculations have been based on either hydrogenic atomic models [2–8] or on numerical Hartree–Slater type calculations for atoms [9–14]. Calculations by Egerton [7] and Luo and Zeitler [8] make use of experimental optical data to calculate cross sections for some elements.

This paper presents a new model for the calculation of innershell excitation cross sections in which the final state of the excited electron is described by a free-electron band rather than the excited state of an atom. Experimental optical data are incorporated into the model in such a way that energy losses involving small momentum transfers are taken into account in a correct manner, i.e. the

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